Eur. Phys. J. Plus (2017) **132**: 243
DOI 10.1140/epjp/i2017-11534-5

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Quasi-four-particle first-order Faddeev-Watson-Lovelace terms in proton-helium scattering*

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Received: 26 December 2016 / Revised: 13 April 2017
Published online: 1 June 2017 –

Abstract. The Faddeev-Watson-Lovelace equations, which are typically used for solving three-particle scattering problems, are based on the assumption of target having one active electron while the other electrons remain passive during the collision process. So, in the case of protons scattering from helium or helium-like targets, in which there are two bound-state electrons, the passive electron has a static role in the collision channel to be studied. In this work, we intend to assign a dynamic role to all the target electrons, as they are physically active in the collision. By including an active role for the second electron in proton-helium–like collisions, a new form of the Faddeev-Watson-Lovelace integral equations is needed, in which there is no disconnected kernel. We consider the operators and the wave functions associated with the electrons to obey the Pauli exclusion principle, as the electrons are indistinguishable. In addition, a quasi-three-particle collision is assumed in the initial channel, where the electronic cloud is represented as a single identity in the collision.

1 Introduction

Many different methods are available in the literature to study the electron capture or charge transfer cross sections [1–13] for the collision of an atom by an ion. This process, in its simplest case, is a three-particle one. However, in general, calculating the charge transfer cross section is a many-particle problem as the target is, at least, a two-particle system. A number of methods have been devised to calculate the single electron capture cross section, including the continuum distorted-wave (CDW) theory [5], the strong potential Born (SPB) approach [4,14], the distorted-wave Born (DWB) method [7], a target continuum distorted-wave (TCDW) theory [8,15], the boundary-corrected first- and second-order Born (B1B and B2B) approximations [9,16], and the impulse approximation [10], which was originally applied to three-particle scattering problems but has now been extended to four-particle scattering problems [17–20].

The perturbative methods based on the Lippmann-Schwinger equation, LS, are devised for the quantum treatment of the charge transfer cross section. The Lippmann-Schwinger integral equation includes a disconnected kernel, resulting in an ambiguity in the solution for a scattering process. Faddeev [1] solved this problem by rearranging the expanded terms in the LS equations. His approach to expanding the LS equation made the formalism by Watson [3] and Lovelace [2] suitable to calculate physical scattering amplitudes, for processes such as a direct collision, breakup and rearrangement processes. This method, known as Faddeev-Watson-Lovelace (FWL) formalism, is a fully quantum mechanical one, where two-particle transition matrices are implemented for the expansion [1–3]. Another, common, expansion is the Born approximation. Here each term of the Faddeev expansion contains an infinite number of terms in a Born series describing a physical sub-reaction involved in the actual scattering process, and in principle giving a full understanding for any reaction. For the electron capture process, Thomas [21] proposed a double scattering mechanism which classically corresponds to a single term in the Faddeev three-particle expansion. Other possible double-scattering mechanisms were considered by Shakeshaft [22] and Briggs [23], which described other terms in the

* Supplementary material in the form of a .pdf file available from the Journal web page at
http://dx.doi.org/10.1140/epjp/i2017-11534-5

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Table 1. Interactions for the two-body channels of a three-particle interaction.

σ	Arrangement	$I(\sigma)$	$E(\sigma)$
1	$P+(TC)$	(TC)	(PC), (PT)
2	$T+(PC)$	(PC)	(TC), (PT)
3	$C+(PT)$	(PT)	(TC), (PC)

second-order FWL terms of the electron transfer process. Although there are limitations in applying the fully quantum-mechanical three-particle Faddeev formalism in an atomic collision system, it is in fact widely applied to calculate the electron capture cross section for fast proton or positron scattering from atoms [6,24–26] or molecules [27,28]. There is some pioneering work on the development of a Faddeev-type formalism to the four-particle scattering case [29–34]. However, the four-particle single charge exchange problem is typically still simplified and treated by the three-particle FWL integral equations [25,26,35]. Usually, an active electron model is devised to study the charge transfer process between the bare ions and a target comprising more than one electron, which is actually a many-particle problem of more than three particles. This model converts from a many-body problem to a three-particle one by assuming there is only one active electron in the target, and that the rest of the target or projectile can be represented as particles. The spin of the electrons is neglected in these types of calculations, where the electrons are assumed to be distinguishable.

2 Fully spin-dependent collisions

For a fully quantum mechanical model based on a LS formalism, such as the four-particle FWL equation, it is not acceptable to neglect the spin of the electrons. Here, we devise a four-particle FWL formalism, as introduced previously [34], for a single charge transfer process in the collision of a bare ion (such as the proton) and a helium-like atom but, now, without neglecting the spin of the electron. We symbolize the interaction as

$$\mathrm{H}^+ + \mathrm{He}(1s^2) \rightarrow \mathrm{H}(1s) + \mathrm{He}^+(1s) \tag{1}$$

or

$$P + (T + e_1 + e_2) \rightarrow (P + e_P) + (T + e_T), \tag{2}$$

where P, T and e are the projectile, the target nucleus and the electrons, respectively. Further note that the electrons on the right-hand side of the above have different indices as compared to those on the left-hand side of the reaction. This is due to the fact that electrons are not distinguishable. e_T and e_P refer to the electron that remains bound to the target and the electron transferred to the projectile, respectively, while 1 and 2 in e_1 and e_2 are just labels for the electrons of the target in the initial channel.

We additionally note here, that, we are adopting the terminology used by Sloan [34]. Sloan makes correct use of the particle and body interactions, where a body may include more than one particle. In a four-particle scattering process, Sloan thus distinguishes four different sets of channels. The first set includes two-body channels of type 1+3, which denotes that one particle is free. There are four channels of this sort, which are labeled by the free particles. We note that in this scheme there are two different two-particle interactions, called internal and external. Internal two-particle interactions are the types between the particles of the bound system, while the external two-particle interactions are those between the free particle and each particle of the bound system. The second set of channels contains three two-body channels of type 2+2, such as an atomic hydrogen-hydrogen interaction. We note that there are seven two-body channels in total. The third set of channels is composed of six three-body channels of type 2+1+1, in which a single pair is bound, while the other two are free, and this set is labeled by the bound pair. An example of type 2+1+1, is the final channel for the ionization of a helium atom by a proton. Finally, there is a four-free-particle channel. Thus, in this scheme, there are fourteen channels available in a general four-body problem. We note that, for each particular channel σ, there are external, $E(\sigma)$, and internal, $I(\sigma)$, two-particle interactions. Those internal and external two-particle interactions are shown in tables 1 and 2 for the three-particle and four-particle interactions, respectively.

According to Sloan [34], a full four-particle T-matrix can be decomposed in the Faddeev manner as

$$T = \sum_{i,j} T_{ji}, \tag{3}$$

where i and j are the initial and final channel labels, respectively, and

$$T_{ji} = \delta_{ji} V_j + V_j G V_i \tag{4}$$

Table 2. The seven two-body channels and their internal interactions for a four-particle interaction.

σ	Arrangement	$I(\sigma)$	$E(\sigma)$
1	$P+(Te_Pe_T)$	(Te_P), (Te_T), (e_Pe_T)	(Pe_P), (Pe_T), (PT)
2	$T+(Pe_Pe_T)$	(Pe_P), (Pe_T), (e_Pe_T)	(Te_P), (Te_T), (PT)
3	$e_P+(PTe_T)$	(PT), (Pe_T), (Te_T)	(Pe_P), (Te_P), (e_Pe_T)
4	$e_T+(PTe_P)$	(PT), (Pe_P), (Te_P)	(e_Pe_T), (Pe_T), (Te_T)
5	$(e_Pe_T)+(PT)$	(e_Pe_T), (PT)	(Pe_T), (Te_T), (Pe_P), (Te_P)
6	$(Pe_T)+(Te_P)$	(Pe_T), (Te_P)	(Pe_P), (Te_T), (e_Pe_T), (PT)
7	$(Pe_P)+(Te_T)$	(Pe_P), (Te_T)	(Pe_T), (Te_P), (e_Pe_T), (PT)

satisfies the Faddeev equations exactly, similarly to the three-particle case, as

$$T_{ji}=\delta_{ji}t_j+\sum_{k\neq j}t_jG_0T_{ki}, \tag{5}$$

where t_j is the two-body T-matrix. Furthermore, G and G_0 are the Green's operators defined, respectively, as

$$G=(E-H_0-V+i\varepsilon)^{-1} \tag{6a}$$

and

$$G_0=(E-H_0+i\varepsilon)^{-1}, \tag{6b}$$

corresponding to the four-particle kinetic operator H_0, the total four-particle energy E, and the total potential operator $V=\sum_i V_i$-where the sum is over all six pairs in the four-particle system. However, in accordance with the three-particle case, the iterated kernel of the Faddeev equations still contains disconnected pieces corresponding with internal scattering interactions in various two-body channels. By introducing $M^\sigma=\sum_{j,i\in I(\sigma)}M^\sigma_{ji}$, for σ ranging over the seven two-body channels, the disconnected kernel problem is solved. This follows as the Faddeev equations are satisfied by M^σ_{ji} as

$$M^\sigma_{ji}=\delta_{ji}t_j+\sum_{k\neq j}t_jG_0M^\sigma_{ki}, \tag{7}$$

where i,j and k are the channel labels and members of $I(\sigma)$. Sloan explained that the multi-scattering interpretation of M^σ_{ji} is that it represents the sum of all internal multiple scattering in the two-body channels, σ, beginning with pair i, while ending with pair j. The part of M^σ_{ji} that is connected with respect to the internal motion in channel σ is

$$\bar{M}^\sigma_{ji}=M^\sigma_{ji}-\delta_{ji}t_j=\sum_{k\neq j}t_jG_0M^\sigma_{ki}\quad\text{for } i,j \text{ and } k\in I(\sigma), \tag{8}$$

while the corresponding operator with no restriction on the first interaction is

$$\bar{M}^\sigma_{j-}=\sum_{i\in I(\sigma)}\bar{M}^\sigma_{ji},\quad\text{for } j\in I(\sigma). \tag{9a}$$

We note that the second order of $\bar{M}^\sigma_{ji}$ is

$$\bar{M}^\sigma_{ji}=t_jG_0t_i(1-\delta_{ji}),\quad\text{for } i \text{ and } j\in I(\sigma). \tag{9b}$$

Finally, as there are no δ functions in the kernel, after the single iteration, it was shown that T_{ji} could be written as

$$T_{ji}=\delta_{ji}t_j+\sum_\sigma\bar{M}^\sigma_{ji}+\sum_\sigma\sum_{k\in E(\sigma)}\bar{M}^\sigma_{j-}G_0T_{ki}, \tag{10}$$

where the disconnected pieces problem in the iterated kernel is now solved. Therefore, the four-body FWL equations for the post (+) and prior (−) forms are obtained as

$$U^\pm_{\beta\alpha}=(1-\delta_{\beta\alpha})\begin{Bmatrix}V_\beta-V_{\beta\alpha}\\V_\alpha-V_{\beta\alpha}\end{Bmatrix}+\sum_{j\in E(\beta)}\sum_{i\in E(\alpha)}T_{ji}, \tag{11}$$

where α and β are the initial and final channels, respectively. Here, for single charge transfer, the α and β channels refer to the interactions, within the two-body types of the form $H^+ + He$ and $H + He^+$, respectively. Additionally, V_α denotes external interactions in the α channel, while $V_{\beta\alpha}$ denotes the interactions that are external to both the α and β channels.

Electrons are fermions of spin 1/2 and so they obey the Pauli exclusion principle as they are indistinguishable. Substituting the electronic cloud identity for the two electrons in atomic helium, we denote the external interactions $E(\alpha)$ in the initial channel as being (PC) and (PT) for the projectile-electronic cloud and the projectile-nucleus interaction, respectively. Here P, T and C stand for the projectile, the target's nucleus and the target's electronic cloud, respectively. The relevant internal and external interactions for a three-particle interaction, which is assumed in the initial channel, are tabulated in table 1.

For a single charge transfer process, the external interactions, $E(\beta)$, in the final channel are given as (PT), (Pe_P), (Te_T) and (e_Te_P). Note that we have made no reference to this for electron 1 or 2 in order to implement their indistinguishability. In addition the external interactions in the α channel, and those in both α and β channels, are given by $V_\alpha = \{V_{PT}, V_{PC}\}$ and $V_{\beta\alpha} = \{V_{PT}\}$, respectively. Thus, making use of relation (11), the terms in the prior form of the FWL transition operators are

$$U^-_{\beta\alpha} = V_{PC} + T_{Pe_T,PC} + T_{Te_P,PC} + T_{e_Pe_T,PC} + T_{PT,PC} + T_{Pe_T,PT} + T_{Te_P,PT} + T_{e_Pe_T,PT} + T_{PT,PT}. \quad (12)$$

In order to expand the FWL terms in relation (12), in terms of the two-body transition matrices, one needs to include all (seven) internal interactions of the two-body channels represented by upper index, σ, which are tabulated in table 2. It is apparent that not all the possible arrangements in table 2 could be described physically, and that they have only mathematical significance which, in practice, contributes minutely in the calculated cross sections.

Making use of Sloan's [34] definition for the particle and body interaction, we will include the electron spin in the calculation only when the target has more than one electron. When a proton interacts with a helium atom, the initial two-body interaction is a 1+3 channel. In our approach we will divide this two-body channel into two interactions. The first represents the proton interaction with the helium nucleus (a particle-particle interaction), while the second is the interaction of the proton with the electron cloud (a particle-body interaction instead of the two interactions of a proton with each electron).

By considering separately the proton-electron cloud interaction, this enables us to include the electron spin into the formalism and guarantee the Pauli exclusion principle. Therefore, the two-body operators for the interaction between a proton, P, and the electron cloud, C, will be

$$t_{PC} = \frac{1}{2}(t_{Pe_P} + t_{Pe_T}) \quad (13)$$

and

$$V_{PC} = \frac{1}{2}(V_{Pe_P} + V_{Pe_T}), \quad (14)$$

where rather than referring to the bound electrons as electron 1 and electron 2, we have used the notation e_P and e_T to denote the electron transferred to the proton (projectile) and the electron left bonded with the helium atom (target), respectively. Additionally, this enables us to formulate a proper connection between the initial channel and the final channel. Making use of the definition

$$T_{j,PC} = \frac{1}{2}(T_{j,Pe_P} + T_{j,Pe_T}), \quad (15)$$

which corresponds with the Pauli exclusion principle, we can expand T_{ji}, in relation with the two-body interaction matrices, t_i. Making use of the operator relations (14) and (15), the prior form of the FWL amplitude (12) is written as

$$\begin{aligned} U^-_{\beta\alpha} = {} & \frac{1}{2}\left(V_{Pe_P} + V_{Pe_T}\right) + T_{Pe_T,PT} + T_{Te_P,PT} + T_{e_Pe_T,PT} + T_{PT,PT} \\ & + \frac{1}{2}\left(T_{Te_P,Pe_P} + T_{Te_P,Pe_T} + T_{Pe_T,Pe_P} + T_{Pe_T,Pe_T}\right) \\ & + \frac{1}{2}\left(T_{e_Pe_T,Pe_P} + T_{e_Pe_T,Pe_T} + T_{PT,Pe_P} + T_{PT,Pe_T}\right). \end{aligned} \quad (16)$$

Employing table 2, we can now expand all the terms of the prior form of the FWL transition operators of eq. (12). The first term, T_{Pe_T,Pe_T}, is found to be

$$T_{Pe_T,Pe_T} = \delta_{Pe_T,Pe_T} t_{Pe_T} + \sum_\sigma \bar{M}^\sigma_{Pe_T,Pe_T} = t_{Pe_T} + \bar{M}^{(2)}_{Pe_T,Pe_T} + \bar{M}^{(3)}_{Pe_T,Pe_T} + \bar{M}^{(6)}_{Pe_T,Pe_T} = t_{Pe_T}, \quad (17)$$

for the final channel when charge exchange between the proton and atomic helium is to be considered. The next terms to be found are

$$T_{Te_P,Pe_T} = \delta_{Te_P,Pe_T} t_{Pe_T} + \sum_{\sigma} \bar{M}^{\sigma}_{Te_P,Pe_T} = t_{Te_P} G_0\, t_{Pe_T}, \tag{18}$$

$$T_{PT,Pe_T} = \delta_{PT,Pe_T} t_{Pe_T} + \sum_{\sigma} \bar{M}^{\sigma}_{PT,Pe_T} = t_{PT} G_0 t_{Pe_T}, \tag{19}$$

$$T_{e_Pe_T,Pe_T} = \delta_{e_Pe_T,Pe_T} t_{Pe_T} + \sum_{\sigma} \bar{M}^{\sigma}_{e_Pe_T,Pe_T} = t_{e_Pe_T} G_0\, t_{Pe_T}, \tag{20}$$

$$T_{Pe_T,Pe_P} = \delta_{Pe_T,Pe_P} t_{Pe_P} + \sum_{\sigma} \bar{M}^{\sigma}_{Pe_T,Pe_P} = t_{Pe_T} G_0\, t_{Pe_P}, \tag{21}$$

$$T_{Te_P,Pe_P} = \delta_{Te_P,Pe_P} t_{Pe_P} + \sum_{\sigma} \bar{M}^{\sigma}_{Te_P,Pe_P} = t_{Te_P} G_0\, t_{Pe_P}, \tag{22}$$

$$T_{PT,Pe_P} = \delta_{PT,Pe_P} t_{Pe_P} + \sum_{\sigma} \bar{M}^{\sigma}_{PT,Pe_P} = t_{PT} G_0\, t_{Pe_P}, \tag{23}$$

$$T_{e_Pe_T,Pe_P} = \delta_{e_Pe_T,Pe_P} t_{Pe_P} + \sum_{\sigma} \bar{M}^{\sigma}_{e_Pe_T,Pe_P} = t_{e_Pe_T} G_0\, t_{Pe_P}, \tag{24}$$

$$T_{Pe_T,PT} = \delta_{Pe_T,PT} t_{PT} + \sum_{\sigma} \bar{M}^{\sigma}_{Pe_T,PT} = t_{Pe_T} G_0\, t_{PT}, \tag{25}$$

$$T_{Pe_P,PT} = \delta_{Tep,PT} t_{PT} + \sum_{\sigma} \bar{M}^{\sigma}_{Tep,PT} = t_{Te_p} G_0\, t_{PT}, \tag{26}$$

$$T_{PT,PT} = \delta_{PT,PT} t_{PT} + \sum_{\sigma} \bar{M}^{\sigma}_{PT,PT} = t_{PT} \tag{27}$$

and

$$T_{e_Pe_T,PT} = \delta_{e_Pe_T,PT} t_{PT} + \sum_{\sigma} \bar{M}^{\sigma}_{e_Pe_T,PT} = t_{e_Pe_T} G_0 t_{PT}. \tag{28}$$

Therefore, the prior form of the FWL transition operators in terms of the two-particle transition matrices are

$$\begin{aligned} U^{-}_{\beta\alpha} = {} & \frac{1}{2}(V_{Pe_P} + V_{Pe_T} + t_{Pe_T}) + t_{PT} + t_{Te_P} G_0 t_{PT} + t_{e_Pe_T} G_0 t_{PT} + t_{Pe_T} G_0 t_{PT} \\ & + \frac{1}{2}(t_{Te_P} + t_{Pe_T} + t_{e_Pe_T} + t_{PT}) G_0 t_{Pe_P} + \frac{1}{2}(t_{Te_P} + t_{e_Pe_T} + t_{PT}) G_0 t_{Pe_T}, \end{aligned} \tag{29}$$

where the Pauli exclusion principle is applied in a four-particle interaction. Details for the derivation of eqs. (17) to (28) are given in the Supplementary Material. Making use of the relation

$$t_{ij} = V_{ij} + V_{ij} G_0 t_{ij}, \tag{30}$$

the prior form of the FWL transition operators now takes the form

$$\begin{aligned} U^{-}_{\beta\alpha} = {} & \frac{1}{2}(V_{Pe_P} + V_{Pe_T} + V_{Pe_T}) + V_{PT} + \frac{1}{2}(t_{Te_P} + t_{Pe_T} + t_{e_Pe_T} + t_{PT}) G_0 t_{Pe_P} \\ & + \frac{1}{2}(V_{Pe_T} + t_{Te_P} + t_{e_Pe_T} + t_{PT}) G_0\, t_{Pe_T} + (t_{Te_P} + t_{e_Pe_T} + t_{Pe_T} + V_{PT}) G_0 t_{PT}. \end{aligned} \tag{31}$$

We call this method a quasi-four-particle treatment, because, in the initial channel, the electronic cloud was assumed to be a single identity (particle), *i.e.* a three-particle system was assumed. However, in the final channel, each electron was represented by a different electronic cloud and therefore, a four-particle system was taken into account. Nonetheless, this classification of the particles does not affect the kernel of the equations and they are connected.

3 Results and conclusion

We now find the first-order FWL transition amplitude, which is similar to the first Born amplitude, as

$$A^{S}_{\mathrm{FWL}} = \left\langle \psi_f \left| \frac{1}{2} V_{Pe_P} + V_{Pe_T} + V_{PT} \right| \psi_i \right\rangle, \tag{32}$$

where the upper index S refers to the spin dependence of the operators. In order to simplify this first-order FWL transition amplitude, we should define the wave functions both before and after the collision.

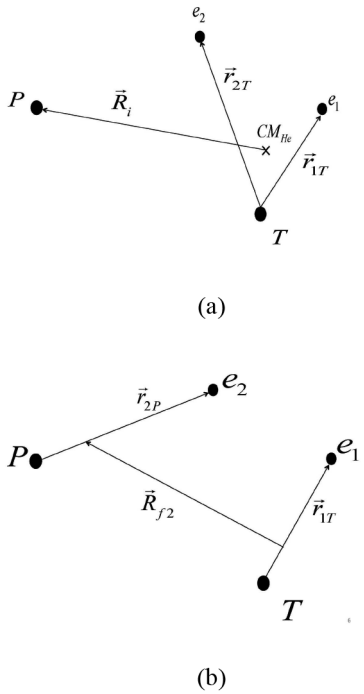

Fig. 1. Jacobi coordinates used to define the wave functions for (a) the initial state and (b) the final state.

The wave functions in the initial and the final channel should be written according to the Pauli exclusion principle, *i.e.* the wave functions should be eigen-functions of the exchange operator. Note that the final comparison between the two treatments will be discussed once the transition amplitudes are simplified.

Applying the Pauli exclusion principle, the initial and the final asymptotic states in position space are

$$\begin{aligned}|\psi_i\rangle &= \psi_i(\vec{r}_1,\vec{r}_2,\vec{R}_i) = \langle\vec{r}_1,\vec{r}_2,\vec{R}_i|i\rangle = \phi_{\mathrm{He}}(\vec{r}_{1T},\vec{r}_{2T})\exp[i\vec{K}_i\cdot\vec{R}_i]\\ &= \phi_{\mathrm{H}1s}(\vec{r}_{1T})\phi_{\mathrm{H}1s}(\vec{r}_{2T})\exp[i\vec{K}_i\cdot\vec{R}_i],\end{aligned} \tag{33}$$

and

$$\begin{aligned}|\psi_f\rangle &= \psi_f(\vec{r}_1,\vec{r}_2,\vec{R}_f) = \langle\vec{r}_1,\vec{r}_2,\vec{R}_f|f\rangle\\ &= \frac{1}{\sqrt{A}}(1\pm P_{12})\phi_{\mathrm{He}^+}(\vec{r}_{2T})\phi_{\mathrm{H}1s}(\vec{r}_{1P})\exp[i\vec{K}_{f_1}\cdot\vec{R}_{f_1}],\end{aligned} \tag{34}$$

respectively, and $\frac{1}{\sqrt{A}}$ is a normalization coefficient. Note that, in eq. (34), the plus and minus signs denote the singlet and triplet states, respectively. $\Phi_{\mathrm{He}}(\vec{r}_{1T},\vec{r}_{2T})$, $\phi_{\mathrm{He}^+}(\vec{r})$, $\phi_{\mathrm{H}1s}(\vec{r}_{1P})$ and $\phi_{\mathrm{H}1s}(\vec{r}_{2T})$ are, in turn, the wave functions for the target atom, singly ionized helium, the hydrogenic wave function formed by the projectile after the collision and the hydrogenic wave function used to define the target atom. The position vectors during the collision are defined by the Jacobi coordinate as shown in fig 1.

Let us now define A_{e_1}, A_{e_2} and A_{PT} as

$$A_{e_1} = \frac{1}{\sqrt{A}}\langle\phi_{\mathrm{He}^+}(\vec{r}_{2T})\phi_{\mathrm{H}}(\vec{r}_{1P})\exp(i\vec{K}_{f_1}\cdot\vec{R}_{f_1})|V_{Pe_1}|\phi_{\mathrm{H}1s}(\vec{r}_{1T})\phi_{\mathrm{H}1s}(\vec{r}_{2T})\exp(i\vec{K}_i\cdot\vec{R}_i)\rangle, \tag{35}$$

$$A_{e_2} = \frac{1}{\sqrt{A}}\langle\phi_{\mathrm{He}^+}(\vec{r}_{2T})\phi_{\mathrm{H}}(\vec{r}_{1P})\exp(i\vec{K}_{f_1}\cdot\vec{R}_{f_1})|V_{Pe_2}|\phi_{\mathrm{H}1s}(\vec{r}_{1T})\phi_{\mathrm{H}1s}(\vec{r}_{2T})\exp(i\vec{K}_i\cdot\vec{R}_i)\rangle \tag{36}$$

and

$$A_{PT} = \frac{1}{\sqrt{A}}\langle\phi_{\mathrm{He}^+}(\vec{r}_{2T})\phi_{\mathrm{H}}(\vec{r}_{1P})\exp(i\vec{K}_{f_1}\cdot\vec{R}_{f_1})|V_{PT}|\phi_{\mathrm{H}1s}(\vec{r}_{1T})\phi_{\mathrm{H}1s}(\vec{r}_{2T})\exp(i\vec{K}_i\cdot\vec{R}_i)\rangle, \tag{37}$$

respectively, to make the coming equations tractable. Note that fig. 2 shows the angular dependence of the amplitudes defined by eqs. (35) to (37). These amplitudes were calculated on a desktop computer and it is relatively straightforward to combine and utilize them (see later) to calculate the cross sections for the scattering process in question. That, in turn, could in principle be compared against relevant results from other theory or measurement.

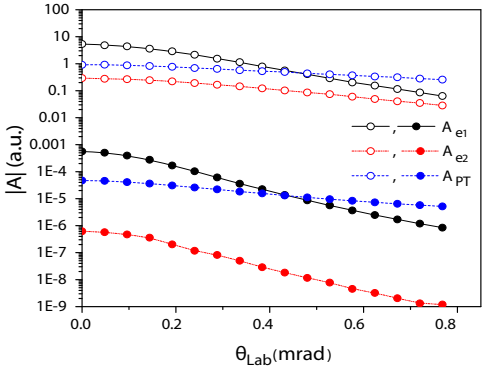

Fig. 2. The angular dependence of the transition amplitudes A_{e1}, A_{e2} and A_{PT}, where the Pauli exclusion principle was applied to the operators. The impact energy is 150 keV for open circles and 7.42 MeV for full circles. Atomic units are chosen.

Now, the FWL transition amplitude, where the Pauli exclusion principle is applied to the operators and wave functions, $A^S_{\rm FWL}$, is

$$A^S_{\rm FWL} = \frac{1}{2}\begin{cases} 3A_{e_1} + 3A_{e_2} + 4A_{PT} & \text{singlet} \\ A_{e_2} - A_{e_1} & \text{triplet}\,. \end{cases} \tag{38}$$

To derive eq. (38), it was assumed that e_T was labeled as electron no. 1 although the result would be the same if e_T was labeled as electron 2. It was also made the correct assumption that $P_{12}V_{PT} = V_{PT}$.

We next define the electronic, A^S_e, and the nuclear, A^S_n, interaction amplitudes which, respectively, are

$$A^S_e = \frac{1}{2}A^S_e\begin{cases} 3A_{e_1} + 3A_{e_2} & \text{singlet} \\ A_{e_2} - A_{e_1} & \text{triplet} \end{cases} \tag{39}$$

and

$$A^S_n = 2\begin{cases} A_{PT} & \text{singlet} \\ 0 & \text{triplet}\,. \end{cases} \tag{40}$$

The results of the current calculations are plotted in fig. 2, at scattering angles of less than 0.8 mrad and for 7.42 MeV (high-energy regime) and 150 keV (medium-energy regime) proton impact energies. The two terms, A_{e1} and A_{PT}, decrease by four orders of magnitude for 7.42 MeV proton impact energy as compared with those at 150 keV impact energy, while the term A_{e2} decreases by six orders of magnitude for similar conditions.

Making use of Sloan's interpretation [34] of the four-particle interaction, but neglecting the Pauli exclusion principle for the operators, the post form of FWL transition operators is

$$\begin{aligned} U^-_{\beta\alpha} = {} & V_{Pe_1} + V_{Pe_2} + V_{PT} + (t_{Te_1} + t_{Pe_2} + t_{e_1e_2} + t_{PT})G_0t_{Pe_1} \\ & + (V_{Pe_2} + t_{Te_1} + t_{e_1e_2} + t_{PT})G_0t_{Pe_2} + (t_{Pe_2} + t_{e_2e_1} + t_{Te_1} + V_{PT})G_0t_{PT}, \end{aligned} \tag{41}$$

which is expressed in terms of the two particle transition matrices and the interaction potential. The difference between relations (31) and (41) is a consequence of taking into account the Pauli exclusion principle for the operators, and making the assumption that there is an electronic cloud both before and after the collision. However, the difference between the operators of eqs. (31) and (41) is not the whole difference between the two treatments.

One can assume the electronic transition amplitude is to be calculated from the terms $V_{Pe_1} + V_{Pe_2}$. Therefore, making use of the same wave functions for the initial and final states, the electronic transition amplitude for the first two terms of eq. (41) takes the form

$$A_e = \langle\psi_f|V_{Pe_1} + V_{Pe_2}|\psi_i\rangle = 2\begin{cases} A_{e_2} + A_{e_1} & \text{singlet} \\ 0 & \text{triplet}\,, \end{cases} \tag{42}$$

where the + and − signs are again for the singlet and triplet cases. The electronic amplitude, eq. (42), does not agree with the result of eq. (38) showing the effect of Pauli exclusion principle being applied to the operators. Note that, here, the spin of the electrons is taken into account for the wavefunctions in both cases.

We can finally calculate the first-order nuclear amplitude term for this case, taking into account the interactions V_{PT}, as

$$A_n = \langle\psi_f|V_{PT}|\psi_i\rangle = 2\begin{cases} A_{PT} & \text{singlet} \\ 0 & \text{triplet}\,, \end{cases} \tag{43}$$

and comparing it with the nuclear term, eq. (40), one concludes that the nuclear term does not change in this model.

Finally, the total amplitude will be

$$A_{\mathrm{FWL}} = A_e + A_n = 2 \begin{cases} A_{e_2} + A_{e_1} + A_{PT} & \text{singlet} \\ 0 & \text{triplet}\,. \end{cases} \tag{44}$$

4 Concluding remarks

In this work, we demonstrated the importance of employing a full quantum treatment in scattering problems, such as charge transfer reactions. A comparison between eqs. (38) and (44) is a consequence of applying the Pauli exclusion principle to the operators. The results of the present calculation are given in fig. 2. The results shown are for two impact energies of 7.42 MeV and 150 keV, where the former is considered to be in the high-energy regime and the latter in the medium-energy regime. The present work is mainly applicable in the high-energy regime, as the incoming proton is assumed to be a plane wave. As one moves to lower energies, this assumption tends not to be so valid. The Coulomb wave describes an incoming proton better for medium energies.

The differences presented here are just for the first-order terms in the LS expansion. This work will now proceed by applying our method up to the second-order terms, and from there to calculate the cross sections to compare with the existing theoretical and experimental results. By including the second-order terms we would expect to find more accurate values for those cross sections.

The authors would like to acknowledge the support of the Research Department of the Graduate University for Advanced Technology, through their grant program. One of us (MJB), also thanks the Australian Research Council for some financial support.

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